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High-pressure IR-spectra and the Thermodynamic Properties of Chloritoid

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Using IR radiation from a synchrotron source, high-quality absorbance spectra were obtained from polycrystalline powder of chloritoid (cld) from ambient conditions up to pressures of 10 GPa over 50 to 4000 cm^{-1} (Fig. 1). The idealized chemical composition of the chloritoid group is $M_2Al_4O_2(SiO_4)_2(OH)_4$ where M = Fe or Mg in our experiments. All of the 42 expected fundamental IR modes were observed. These data, combined with the response of the IR bands to substitutions of Fe for Mg, and of D for H, constrained the band assignments. Heat capacity (C_P) and entropy (S_O) for the triclinic and monoclinic polymorphs of Fe- and Mg-cld were calculated from Kieffer-type model, using our detailed band assignments. The calculated heat capacity and entropy for the monoclinic and triclinic polymorphs differ negligibly. The results at temperatures of above 298 K are described by the following polynomial expressions in J/mol-K: $C_P = 7.835*10^2-5.170*10^3T^{-0.5}- 1.648*10^7T^{-2}+1.934*10^9T^{-3}$ for Mg-cld and $C_P = 7.848*10^2-5.185*10^3T^{-0.5}- 1.548*10^7T^{-2}+1.783*10^9T^{-3}$ for Fe-cld. At room temperature, S_O = 293 J/mol-K for Mg-cld and 335 J/mol-K for Fe-cld. Using these values in conjunction with the enthalpy of formation, H_f = -7101 kJ/mol for Mg-cld or H_f =-6422 kJ/mol for Fe-cld (estimated in this study), we can closely reproduce the experimental data for the reactions Mg-chloritoid+talc = clinochlore+kyanite (Chopin 1985) and Fe-chloritoid = almandine+diaspore+water (Vidal et al. 1994).

References:

(1) C. Chopin “Les relations de phases dans les metapelites de houte pression”. PHD Thesis. Mém. Sc. Terre Univ. Curie, Paris, no. 85-11, 1985

(2) O. Vidal, T. Theye, and C. Chopin “Experimental study of chloritoid stability at high pressure and various f_{O2} conditions”. Con. Min. Petrol., **118**, *256-270*, 1994

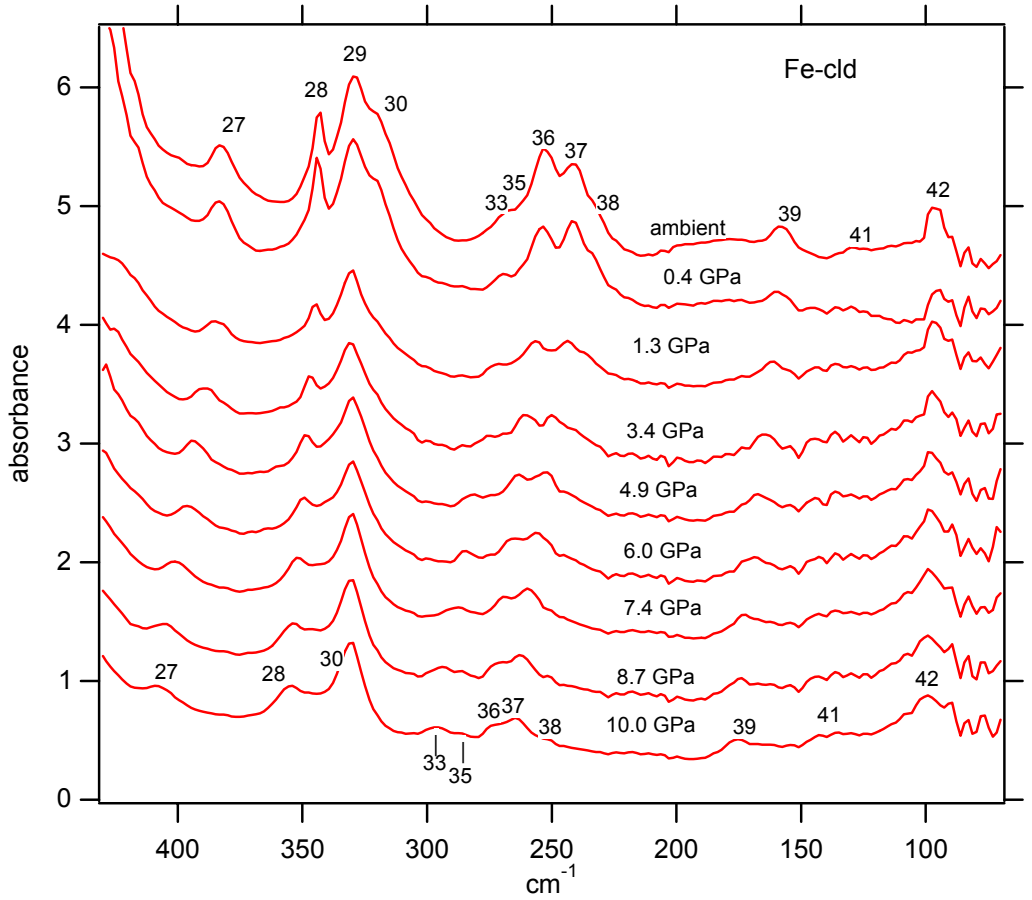

Fig. 1: Far-IR spectra of Fe-chloritoid at different pressures. The spectra are offset for clarity.